

=> file reg

FILE 'REGISTRY' ENTERED AT 13:34:52 ON 01 DEC 2003
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STRUCTURE FILE UPDATES: 30 NOV 2003 HIGHEST RN 622330-21-6
DICTIONARY FILE UPDATES: 30 NOV 2003 HIGHEST RN 622330-21-6

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STN Note 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> file caplus

FILE 'CAPLUS' ENTERED AT 13:34:55 ON 01 DEC 2003
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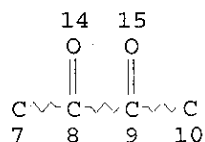
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FILE COVERS 1907 - 1 Dec 2003 VOL 139 ISS 23
FILE LAST UPDATED: 30 Nov 2003 (20031130/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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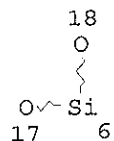
L1 STR



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 6

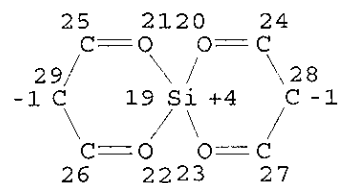
STEREO ATTRIBUTES: NONE
 L2 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE
 L3 (5)SEA FILE=REGISTRY SSS FUL L1 AND L2
 L4 (1)SEA FILE=REGISTRY ABB=ON PLU=ON 366803-70-5
 L5 (1)SEA FILE=REGISTRY ABB=ON PLU=ON 366803-71-6
 L6 STR



NODE ATTRIBUTES:
 CHARGE IS E+4 AT 19
 CHARGE IS E-1 AT 28
 CHARGE IS E-1 AT 29
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L7 (211)SEA FILE=REGISTRY SSS FUL L6
L8 (2)SEA FILE=CAPLUS ABB=ON PLU=ON L4
L9 (1)SEA FILE=CAPLUS ABB=ON PLU=ON L5
L10 (3)SEA FILE=CAPLUS ABB=ON PLU=ON L3
L11 (67)SEA FILE=CAPLUS ABB=ON PLU=ON L7
L12 (1665919)SEA FILE=CAPLUS ABB=ON PLU=ON (C23C00?/IC OR TRANSITION
METAL? OR KETONES? OR VAPOR DEPOSITION? OR MOS CAPACITOR?)/IT
OR ELECTRIC?
L13 (12)SEA FILE=CAPLUS ABB=ON PLU=ON L12 AND (L10 OR L11)
L14 (9)SEA FILE=CAPLUS ABB=ON PLU=ON L12 AND (L10 OR L11) AND (L8
OR L9 OR SI OR SILIC? OR SIO2)
L15 12 SEA FILE=CAPLUS ABB=ON PLU=ON L13 OR L14

=> d ti 1-12

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI Ultrathin zirconium **silicate** films deposited on Si
(100) using Zr(Oi-Pr)₂(thd)₂, Si(Ot-Bu)₂(thd)₂, and nitric oxide

L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI Photolytic conversion process to form patterned amorphous film

L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI **Silicon** reagents and low temperature CVD method of forming
silicon-containing gate dielectric materials using same

L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI Manufacture of electrophotographic photoreceptor without structure defects

L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI Thermal and **electrical** studies of **silicon**
phthalocyanine dichloride and tris(2,4-pentanedionato)**silicon**
chloride hydrochloride

L15 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI Structural, thermal and **electrical** studies of complexes of
silicon with some first row transition elements

L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
TI Syntheses and **electrical** properties of TCNQ^{•-} radical anion
salts of some tris(β-diketonato) **siliconium**(IV) cations and
x-ray crystal structure of the 1:2 salt of tris(acetylacetonato)
siliconium(IV) with TCNQ

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

- TI **Electric**-field effects in nuclear magnetic resonance spectroscopy. III. ^{13}C -- ^1H spin-spin coupling constants
- L15 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
- TI **Electric** field effects in magnetic resonance. I. Carbon- 13 chemical shifts
- L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
- TI Ring currents in metal acetylacetonates. **Electric** field effects on the proton resonances of cationic and anionic β -diketonate complexes
- L15 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
- TI Preparation and properties of some six- and seven-coordinate halo(acetylacetonato) complexes of zirconium(IV) and hafnium(IV)
- L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
- TI Nuclear magnetic resonance spectra of some β -diketone complexes of Groups III and IV elements

=> d ibib abs hitstr ind total

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:458503 CAPLUS

DOCUMENT NUMBER: 139:205554

TITLE: Ultrathin zirconium **silicate** films deposited on $\text{Si}(100)$ using $\text{Zr}(\text{O}i\text{-Pr})_2(\text{thd})_2$, $\text{Si}(\text{O}t\text{-Bu})_2(\text{thd})_2$, and nitric oxide

AUTHOR(S): Chen, H.-W.; Huang, T.-Y.; Landheer, D.; Wu, X.; Moisa, S.; Sproule, G. I.; Kim, J. K.; Lennard, W. N.; Chao, T.-S.

CORPORATE SOURCE: Institute of Electronics Engineering, National Chiao-Tung University, Hsinchu, 300, Taiwan

SOURCE: Journal of the Electrochemical Society (2003), 150(7), C465-C471

CODEN: JESOAN; ISSN: 0013-4651

PUBLISHER: Electrochemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Ultrathin Zr **silicate** films were deposited using $\text{Zr}(\text{O}i\text{-Pr})_2(\text{tetramethylheptanedione, thd})_2$, $\text{Si}(\text{O}t\text{-Bu})_2(\text{thd})_2$ and nitric oxide in a pulse-mode metalorg. chemical-vapor deposition apparatus with a liquid injection source. High-resolution transmission electron microscopy, atomic force microscopy, XPS, and medium energy ion scattering were employed to investigate the structure, surface roughness, chemical state, and composition of the films. The nitric oxide used as oxidizing gas, instead of O_2 , not only reduced the thickness of the interfacial layer but also removed the carbon contamination effectively from the bulk of the films. The

as-deposited Zr silicate films with a Si:Zr ratio of 1.3:1 were amorphous, with an amorphous interfacial layer 0.3-0.6 nm thick. After a spike anneal in oxygen and a 60 s nitrogen anneal at 850°, these films remained amorphous throughout without phase separation, but the interfacial layer increased in thickness. No evidence of Zr-C and Zr-Si bonds were found in the films by XPS, and carbon concns. <0.1 atom %, the detection limit, were obtained. The hysteresis, fixed charge d., and leakage current determined from capacitance-voltage anal. improved significantly after postdeposition anneals at 850°, and the films exhibited promising characteristics for deep submicrometer metal-oxide-semiconductor devices.

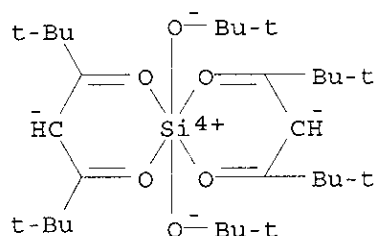
IT 366803-70-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(Si(Ot-Bu)₂(thd)₂; ultrathin zirconium silicate films deposited on Si(100))

RN 366803-70-5 CAPLUS

CN Silicon, bis(2-methyl-2-propanolato)bis(2,2,6,6-tetramethyl-3,5-heptanedionato-κO,κO')-, (OC-6-21)-(9CI) (CA INDEX NAME)



CC 76-2 (Electric Phenomena)

ST MOCVD ultrathin zirconium silicate film

IT Vapor deposition process

(metalorg.; ultrathin zirconium silicate films deposited on Si(100))

IT Ultrathin films

(ultrathin zirconium silicate films deposited on Si(100))

IT 366803-70-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(Si(Ot-Bu)₂(thd)₂; ultrathin zirconium silicate films deposited on Si(100))

IT 204522-78-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(Zr(Oi-Pr)₂(thd)₂; ultrathin zirconium silicate films deposited on Si(100))

IT 7440-21-3, Silicon, uses

RL: NUU (Other use, unclassified); USES (Uses)

(ultrathin zirconium silicate films deposited on Si(100))

IT 10102-43-9, Nitric oxide, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(ultrathin zirconium silicate films deposited on Si
(100))

IT 10101-52-7, Zirconium silicate

RL: TEM (Technical or engineered material use); USES (Uses)

(ultrathin zirconium silicate films deposited on Si
(100))

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:241804 CAPLUS

DOCUMENT NUMBER: 138:247151

TITLE: Photolytic conversion process to form patterned
amorphous film

INVENTOR(S): Bravo-Vasquez, Juan-Pablo; Hill, Ross H.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 23 pp., Cont.-in-part of U.S.
Ser. No. 37,176.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003059544	A1	20030327	US 2002-263701	20021004
US 6348239	B1	20020219	US 2000-561744	20000428
US 2002068188	A1	20020606	US 2001-37176	20011108
US 2002134963	A1	20020926	US 2001-7134	20011204
WO 2003031682	A2	20030417	WO 2002-US31683	20021004
WO 2003031682	A3	20030828		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-561744 A3 20000428
US 2001-327009P P 20011005
US 2001-37176 A2 20011108
US 1998-92024P P 19980706
US 1999-343532 A3 19990630

OTHER SOURCE(S): MARPAT 138:247151

AB The invention is directed to a photoresist-free method for depositing
films composed of metals, such as Cu or SiO₂, or their oxides
from metal complexes. More specifically, the method involves applying an
amorphous film of a metal complex to a substrate. The metal complexes

have a metal and a photo-degradable ligand. A preferred ligand is acac or alkyl-acac, especially in combination with acetate ligands. These films, upon, e.g., thermal, photochem. or electron beam irradiation may be converted to the metal or its oxides. By using either directed light or electron beams, this may lead to a patterned metal or metal oxide film in a single step. Low temperature baking may be used to remove residual orgs. from the deposited film. If SiO₂ is the metal, the deposited film has excellent smoothness and dielec. properties.

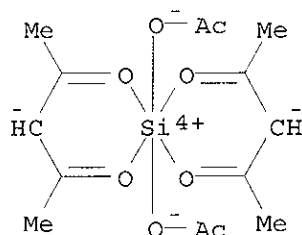
IT 74431-00-8 501417-59-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(photolytic conversion process to form patterned amorphous film)

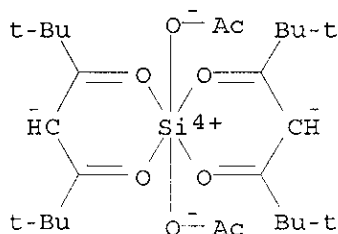
RN 74431-00-8 CAPLUS

CN Silicon, bis(acetato- κ O)bis(2,4-pentanedionato- κ O, κ O')-,
(OC-6-11)- (9CI) (CA INDEX NAME)



RN 501417-59-0 CAPLUS

CN Silicon, bis(acetato- κ O)bis(2,2,6,6-tetramethyl-3,5-heptanedionato- κ O, κ O')-, (OC-6-11)- (9CI) (CA INDEX NAME)



IC ICM B05D003-06

NCL 427385500; 427508000; 427496000; 427504000; 427510000

CC 76-12 (Electric Phenomena)

Section cross-reference(s): 78

ST photolytic conversion coating process amorphous film

IT Alcohols, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(amino; photolytic conversion process to form patterned amorphous film)

IT Films

(amorphous; photolytic conversion process to form patterned amorphous film)

IT Coating process
(electron-beam; photolytic conversion process to form patterned amorphous film)

IT Electron beams
(irradiation; photolytic conversion process to form patterned amorphous film)

IT Coating process
(photochem.; photolytic conversion process to form patterned amorphous film)

IT Dielectric films
Photolysis
(photolytic conversion process to form patterned amorphous film)

IT Transition metal complexes
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolytic conversion process to form patterned amorphous film)

IT Hydroxides (inorganic)
Oxides (inorganic), uses
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(photolytic conversion process to form patterned amorphous film)

IT 74431-00-8 140914-00-7 372112-18-0 372112-19-1
501417-59-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolytic conversion process to form patterned amorphous film)

IT 372112-15-7P, Copper uranium oxide
RL: SPN (Synthetic preparation); PREP (Preparation)
(photolytic conversion process to form patterned amorphous film)

IT 7440-50-8P, Copper, uses 7631-86-9P, Silica, uses
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(photolytic conversion process to form patterned amorphous film)

L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:781198 CAPLUS

DOCUMENT NUMBER: 135:312090

TITLE: Silicon reagents and low temperature CVD
method of forming silicon-containing gate
dielectric materials using same

INVENTOR(S): Xu, Chongying; Baum, Thomas H.; Hendrix, Bryan C.

PATENT ASSIGNEE(S): Advanced Technology Materials, Inc., USA

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001079578	A1	20011025	WO 2001-US11476	20010409
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ,				

LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL,
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US,
UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-551018 A 20000418

AB Si chemical vapor deposition precursors are presented for forming Si films. Hexa-coordinated Si beta-diketonate compns. are described, $R_2Si(-diketonate)_2$ or $(RO)_2Si(\beta-diketonate)_2$, in which each R is the same as or different from the other R, and each R is independently selected from H, aryl, fluoroaryl, C1-C12 alkyl, C1-C12 fluoroalkyl and C1-C12 Si-containing alkyl. The precursors are compatible with dopant co-precursors such as transition metal β -diketonate coordination complexes. The compns. enable low temperature (e.g., $<600^\circ$) formation of gate dielects., capacitor films, etc., in the fabrication of VLSI microelectronic devices.

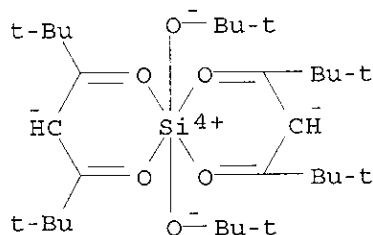
IT 366803-70-5P 366803-71-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(silicon reagents and low temperature CVD method of forming silicon-containing gate dielec. materials using same)

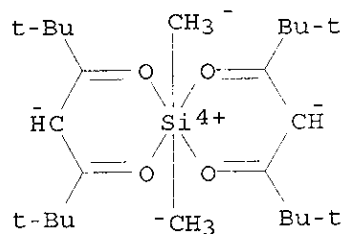
RN 366803-70-5 CAPLUS

CN Silicon, bis(2-methyl-2-propanolato)bis(2,2,6,6-tetramethyl-3,5-heptanedionato- $\kappa O, \kappa O'$)-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 366803-71-6 CAPLUS

CN Silicon, dimethylbis(2,2,6,6-tetramethyl-3,5-heptanedionato- $\kappa O, \kappa O'$)-, (OC-6-21)- (9CI) (CA INDEX NAME)



IC ICM C23C008-00
ICS C23C016-00

CC 76-2 (Electric Phenomena)
Section cross-reference(s): 75

ST **silicon** beta diketonate chem vapor deposition precursor

IT **Transition metal** complexes
RL: RCT (Reactant); RACT (Reactant or reagent)
(1,3-diketone complexes, **vapor deposition**
precursors; **silicon** reagents and low temperature CVD method of
forming **silicon**-containing gate dielec. materials using same)

IT **Ketones**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(1,3-diketones, **transition metal** complexes,
vapor deposition precursors; **silicon**
reagents and low temperature CVD method of forming **silicon**-containing
gate dielec. materials using same)

IT **Vapor deposition** process
(chemical, low-temperature; **silicon** reagents and low temperature CVD method
of forming **silicon**-containing gate dielec. materials using same)

IT **MOS capacitors**
(complementary; **silicon** reagents and low temperature CVD method of
forming **silicon**-containing gate dielec. materials using same)

IT Capacitors
Dielectric films
Integrated circuits
Semiconductor device fabrication
(**silicon** reagents and low temperature CVD method of forming
silicon-containing gate dielec. materials using same)

IT 7440-21-3, **Silicon**, processes 7631-86-9, **Silica**,
processes 11105-01-4, **Silicon** nitride oxide
RL: DEV (Device component use); PEP (Physical, engineering or chemical
process); TEM (Technical or engineered material use); PROC (Process); USES
(Uses)
(**silicon** reagents and low temperature CVD method of forming
silicon-containing gate dielec. materials using same)

IT 366803-70-5P 366803-71-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(**silicon** reagents and low temperature CVD method of forming
silicon-containing gate dielec. materials using same)

IT 111-65-9, Octane, miscellaneous
RL: MSC (Miscellaneous)
(**vapor deposition** precursor solvent;
silicon reagents and low temperature CVD method of forming
silicon-containing gate dielec. materials using same)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:808156 CAPLUS
DOCUMENT NUMBER: 123:213174
TITLE: Manufacture of electrophotographic photoreceptor

without structure defects
 INVENTOR(S): Yamazaki, Koji; Ebara, Toshuki; Ueda, Shigenori;
 Niino, Hiroaki; Kawada, Masaya
 PATENT ASSIGNEE(S): Canon Kk, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07183548	A2	19950721	JP 1993-326948	19931224

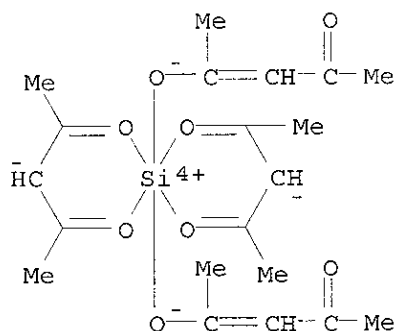
PRIORITY APPLN. INFO.: JP 1993-326948 19931224

AB Manufacture of the photoreceptor includes laminating a hydrogenated α -Si photoconductive layer on an elec. conductive support, coating a sol polymer dispersion containing an organic metal compound, water, an alc., and an acid on the photoconductive layer, gelling the sol polymer dispersion by hydrolysis or polymerization, and removing water and alc. by heating to form a metal oxide layer.

IT 168062-21-3
 RL: TEM (Technical or engineered material use); USES (Uses)
 (contained in sol polymer dispersion for forming metal oxide layer of photoreceptor)

RN 168062-21-3 CAPLUS

CN Silicon, bis(4-hydroxy-3-penten-2-onato-O4)bis(2,4-pentanedionato-O,O')-(9CI) (CA INDEX NAME)



IC ICM H01L031-0248
 CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 ST electrophotog photoreceptor manuf metal oxide layer
 IT Electrophotographic photoconductors and photoreceptors
 (manufacture of metal oxide layer for)
 IT 78-10-4 546-68-9, Tetraisopropoxy Titanium 681-84-5 18267-08-8,
 Tetraethoxy Zirconium 168062-21-3

RL: TEM (Technical or engineered material use); USES (Uses)
(contained in sol polymer dispersion for forming metal oxide layer of
photoreceptor)

L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:244934 CAPLUS

DOCUMENT NUMBER: 112:244934

TITLE: Thermal and electrical studies of
silicon phthalocyanine dichloride and
tris(2,4-pentanedionato)silicon chloride
hydrochloride

AUTHOR(S): Allan, J. R.; Paton, A. D.; Turvey, K.; Gerrard, D.
L.; Hoey, S.

CORPORATE SOURCE: Dep. Appl. Chem. Sci., Napier Polytec., Edinburgh, UK

SOURCE: Thermochimica Acta (1989), 155, 203-10

CODEN: THACAS; ISSN: 0040-6031

DOCUMENT TYPE: Journal

LANGUAGE: English

AB TG and DTA studies were carried out on Si(acac)₃Cl.HCl (Hacac =
acetylacetone) and SiPcCl₂ (H₂Pc = phthalacyanine). Si
(acac)₃Cl.HCl undergoes an endothermic reaction with loss of HCl to give
Si(acac)₃Cl. Si(acac)₃Cl and SiPcCl₂ both undergo
exothermic reactions with loss of the organic ligand and halogen to give
SiO₂. All of the materials exhibit a small departure from Ohm's
law which is attributed to space charge effects. Under a field of 1
+ 10⁴ V m⁻¹, the conductivities are 7 + 10⁻⁸-1.5 + 10⁻⁷
Ω⁻¹ m⁻¹. The temperature dependence of conductivity is anomalous.

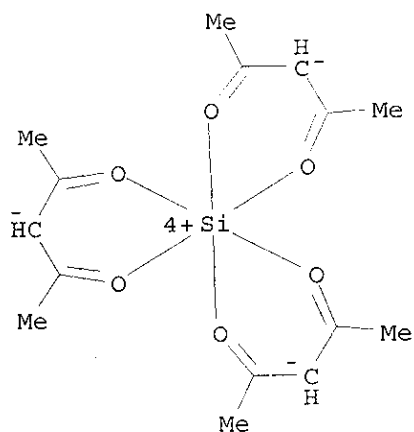
IT 19552-36-4P, Tris(acetylacetonato)silicon(1+)
monochloride

RL: PRP (Properties); PREP (Preparation)

(formation from hydrochloride and thermal decomposition and elec.
conductivity of)

RN 19552-36-4 CAPLUS

CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, chloride, (OC-6-11)- (9CI)
(CA INDEX NAME)



IT 16871-35-5, Tris(acetylacetonato)silicon(1+)
monochloride monohydrochloride

RL: PRP (Properties)

(thermal decomposition and elec. conductivity of)

RN 16871-35-5 CAPLUS

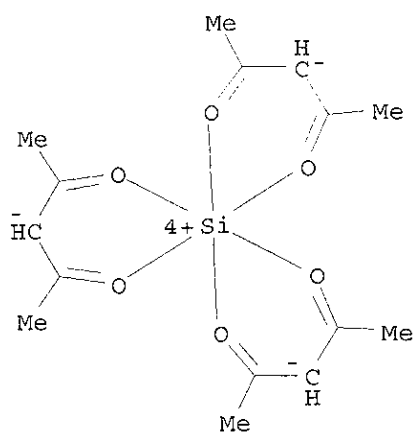
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, (hydrogen
dichloride) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS



KOROMA EIC1700

CM 2

CRN 23231-72-3

CMF Cl2 H

$^{-}\text{Cl}-\text{H}^{+}\text{Cl}^{-}$

- CC 78-9 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 76
- ST thermal decompn **silicon** acetylacetonato phthalocyaninato complex; **elec** cond **silicon** acetylacetonato phthalocyananinato complex; **silicon** acetylacetonato phthalocyaninato thermolysis **elec** cond
- IT **Electric** conductivity and conduction
(of **silicon** acetylacetonato or phthalocyaninato complexes)
- IT 19552-36-4P, Tris(acetylacetonato)**silicon**(1+) monochloride
RL: PRP (Properties); PREP (Preparation)
(formation from hydrochloride and thermal decomposition and **elec.** conductivity of)
- IT 16871-35-5, Tris(acetylacetonato)**silicon**(1+) monochloride monohydrochloride 19333-10-9, Dichloro(phthalocyaninato)**silicon**
RL: PRP (Properties)
(thermal decomposition and **elec.** conductivity of)

L15 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:29781 CAPLUS

DOCUMENT NUMBER: 112:29781

TITLE: Structural, thermal and **electrical** studies of complexes of **silicon** with some first row transition elements

AUTHOR(S): Allan, J. R.; Paton, A. D.; Turvey, K.; Gerrard, D. L.; Hoey, S.

CORPORATE SOURCE: Dep. Appl. Chem. Sci., Napier Polytech., Edinburgh, UK

SOURCE: Thermochemica Acta (1989), 146, 317-27

CODEN: THACAS; ISSN: 0040-6031

DOCUMENT TYPE: Journal

LANGUAGE: English

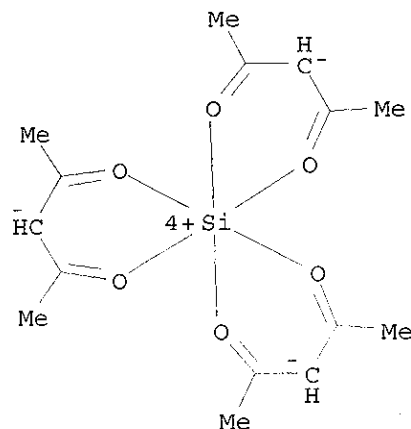
AB [Si(acac)3]MCl3 (Hacac = acetylacetone; M = Co, Cu, Zn) and [Si(acac)3]FeCl4 were prepared from [Si(acac)3]Cl.HCl, prepared from SiCl4 and Hacac, and the resp. metal chlorides. The vibrational and electronic spectra and some magnetic properties are reported for the compds. The thermal behavior of each compound was studied using thermogravimetry. A mixed metal oxide is formed on decomposition for each compound **Elec.** measurements are reported, including detns. of the conductivity and activation energy. For the Zn complex the room temperature conductivity is sufficiently high that device applications are a possibility.

IT 19552-36-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reactions of, with transition metal
chlorides)

RN 19552-36-4 CAPLUS

CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, chloride, (OC-6-11)- (9CI)
(CA INDEX NAME)



● Cl⁻

IT 17348-25-3P 19680-74-1P 124366-29-6P
124366-30-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and thermal decomposition and IR spectrum and elec.
conductivity
of)

RN 17348-25-3 CAPLUS

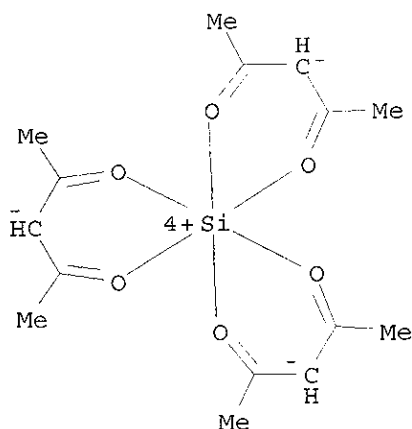
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-,
(T-4)-tetrachloroferrate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS

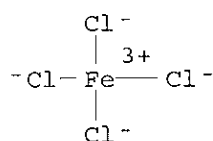


CM 2

CRN 14946-92-0

CMF Cl4 Fe

CCI CCS



RN 19680-74-1 CAPLUS

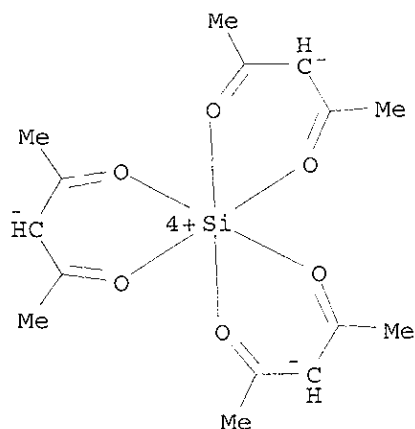
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, trichlorozincate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS

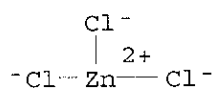


CM 2

CRN 23603-98-7

CMF C13 Zn

CCI CCS



RN 124366-29-6 CAPLUS

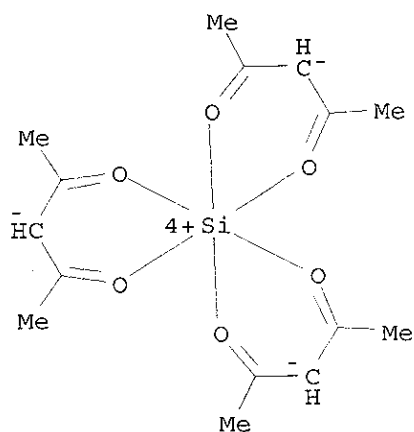
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, trichlorocobaltate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS

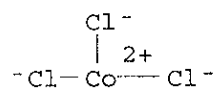


CM 2

CRN 18904-74-0

CMF C13 Co

CCI CCS



RN 124366-30-9 CAPLUS

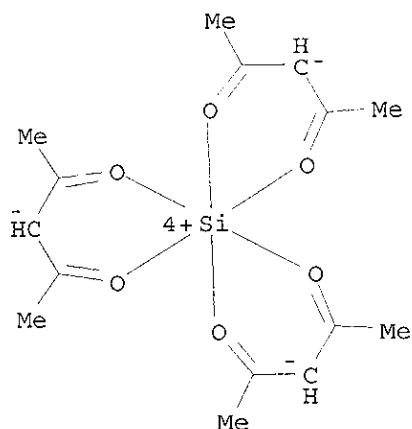
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, trichlorocuprate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS

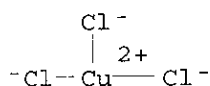


CM 2

CRN 15697-18-4

CMF Cl3 Cu

CCI CCS



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 76

ST thermal decompn **silicon** acetylacetonato chlorometallate; ferrate
chloro **silicon** acetylacetonato; zincate chloro **silicon**
acetylacetonato; cobaltate chloro **silicon** acetylacetonato;
cuprate chloro **silicon** acetylacetonato; elec cond
silicon acetylacetonato chlorozincate

IT **Electric** conductivity and conduction

Infrared spectra

Thermal decomposition

(of **silicon** acetylacetonato complex salts with
chlorometalates)

IT **Transition metals**, compounds

RL: SPN (Synthetic preparation); PREP (Preparation)

(complexes, **silicon**-containing acetato chloro, preparation and thermal
decomposition and elec. conductivity of)

IT 123-54-6, Acetylacetone, properties

RL: PRP (Properties)

(IR spectrum of)

IT **19552-36-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and reactions of, with transition metal
chlorides)

IT 17348-25-3P 19680-74-1P 124366-29-6P
124366-30-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and thermal decomposition and IR spectrum and elec.
conductivity
of)

L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:471373 CAPLUS

DOCUMENT NUMBER: 103:71373

TITLE: Syntheses and electrical properties of
TCNQ•- radical anion salts of some
tris(β-diketonato) siliconium(IV)
cations and x-ray crystal structure of the 1:2 salt of
tris(acetylacetonato)siliconium(IV) with
TCNQ

AUTHOR(S): Ueyama, Kosuke; Matsubayashi, Genetsu; Shimohara,
Ichiro; Tanaka, Toshio; Nakatsu, Kazumi

CORPORATE SOURCE: Dep. Appl. Chem., Osaka Univ., Osaka, 565, Japan

SOURCE: Journal of Chemical Research, Synopses (1985), (2),
48-9

CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:71373

AB Seven salts of the TCNQ radical anion (I•-) with [Si
[CR(COR1)2]3]+ (II; R = H, R1 = Me, CMe3, Ph; R = Et, R1 = Me) were
prepared, and their elec. resistivities examined II.(I•-)2 (R =
H, R1 = Me) exists in monoclinic and triclinic forms, the structures of
which were determined by x-ray anal. In the monoclinic form, the TCNQ mols.
stack in columns along the b axis; adjacent columns form sheets parallel
to the bc plane, and successive sheets are separated along the a axis by the
cationic species.

IT 97501-23-0P 97501-26-3P 97501-27-4P
97501-29-6P 97501-30-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and elec. resistivity of)

RN 97501-23-0 CAPLUS

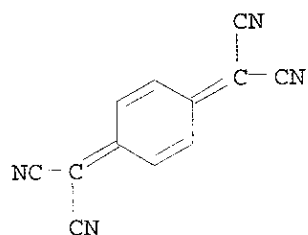
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, salt with
2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 34507-61-4

CMF C12 H4 N4

CCI RIS

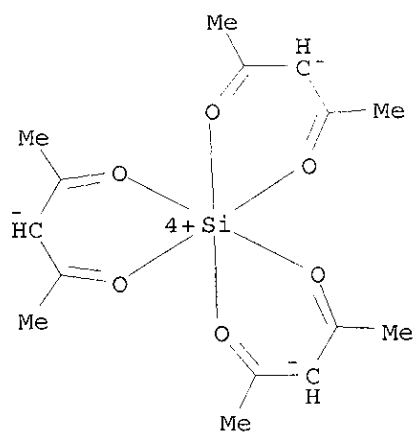


CM 2

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS



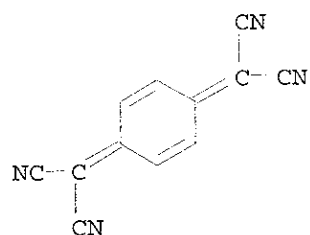
RN 97501-26-3 CAPLUS

CN Silicon(1+), tris(3-ethyl-2,4-pentanedionato-O,O')-, (OC-6-11), salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 1518-16-7

CMF C12 H4 N4



CM 2

CRN 97501-25-2

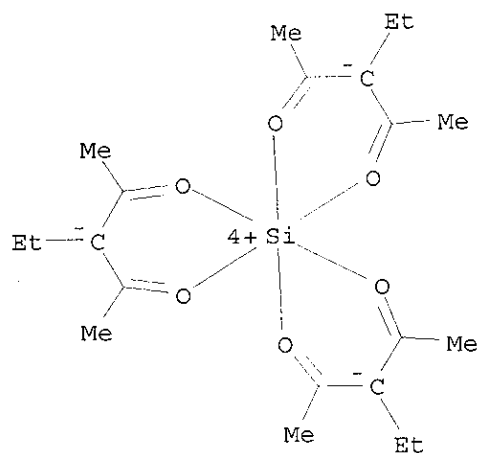
CMF C21 H33 O6 Si . C12 H4 N4

CM 3

CRN 47559-76-2

CMF C21 H33 O6 Si

CCI CCS

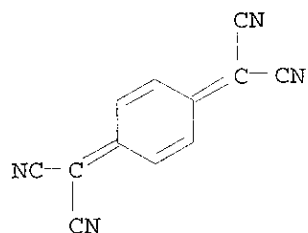


CM 4

CRN 34507-61-4

CMF C12 H4 N4

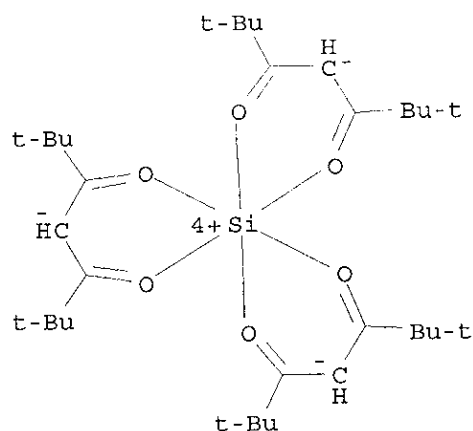
CCI RIS



RN 97501-27-4 CAPLUS
 CN Silicon(1+), tris(2,2,6,6-tetramethyl-3,5-heptanedionato-O,O')-,
 (OC-6-11)-, salt with 2,2'-(2,5-cyclohexadiene-1,4-
 diylidene)bis[propanedinitrile] (1:1) (9CI) (CA INDEX NAME)

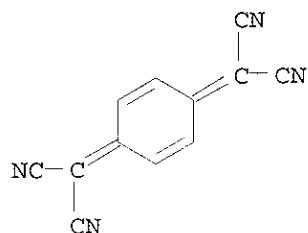
CM 1

CRN 73881-83-1
 CMF C33 H57 O6 Si
 CCI CCS



CM 2

CRN 34507-61-4
 CMF C12 H4 N4
 CCI RIS

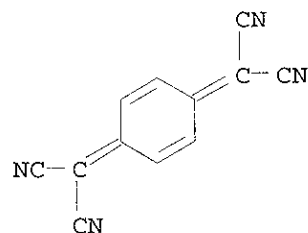


RN 97501-29-6 CAPLUS
 CN Silicon(1+), tris(1,3-diphenyl-1,3-propanedionato-O,O')-, (OC-6-11)-, salt
 with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:2)
 (9CI) (CA INDEX NAME)

CM 1

CRN 1518-16-7

CMF C12 H4 N4



CM 2

CRN 97501-28-5

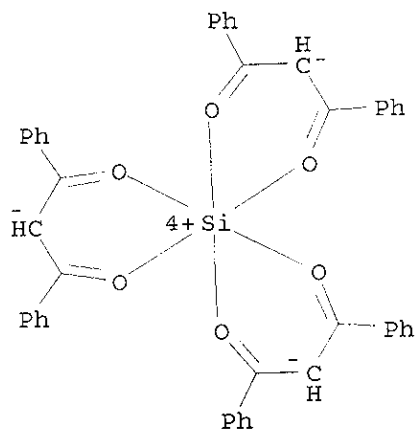
CMF C45 H33 O6 Si . C12 H4 N4

CM 3

CRN 47882-79-1

CMF C45 H33 O6 Si

CCI CCS

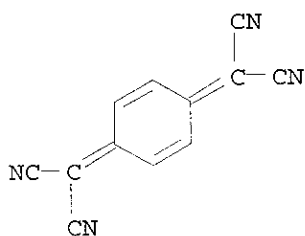


CM 4

CRN 34507-61-4

CMF C12 H4 N4

CCI RIS



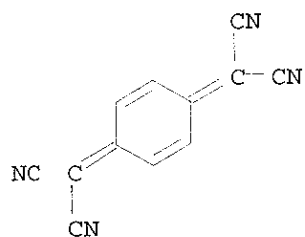
RN 97501-30-9 CAPLUS

CN Silicon(1+), tris(1,3-diphenyl-1,3-propanedionato-O,O')-, (OC-6-11)-, salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (2:5) (9CI) (CA INDEX NAME)

CM 1

CRN 1518-16-7

CMF C12 H4 N4



CM 2

CRN 97501-28-5

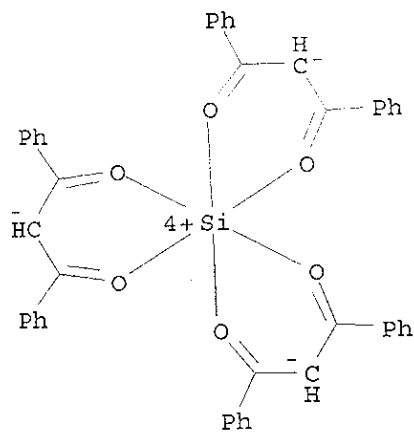
CMF C45 H33 O6 Si . C12 H4 N4

CM 3

CRN 47882-79-1

CMF C45 H33 O6 Si

CCI CCS

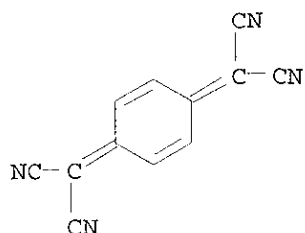


CM 4

CRN 34507-61-4

CMF C12 H4 N4

CCI RIS



IT 97501-24-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, **elec.** resistivity, and crystal and mol. structure of
2 crystalline forms of)

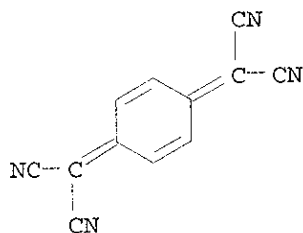
RN 97501-24-1 CAPLUS

CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, salt with
2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:2) (9CI)
(CA INDEX NAME)

CM 1

CRN 1518-16-7

CMF C12 H4 N4



CM 2

CRN 97501-23-0

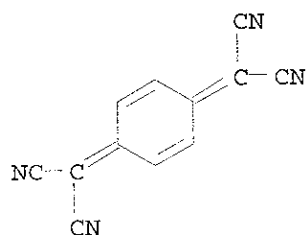
CMF C15 H21 O6 Si . C12 H4 N4

CM 3

CRN 34507-61-4

CMF C12 H4 N4

CCI RIS

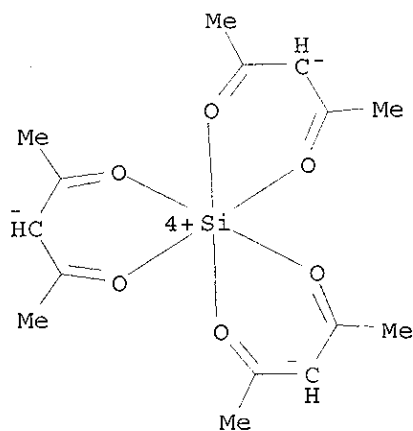


CM 4

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS



IT 97501-28-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, elec. resistivity, and reaction of, with TCNQ)

RN 97501-28-5 CAPLUS

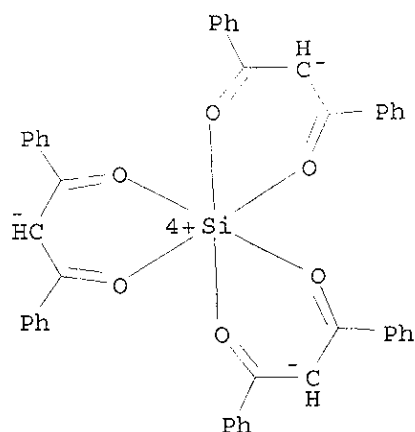
CN Silicon(1+), tris(1,3-diphenyl-1,3-propanedionato-O,O')-, (OC-6-11)-, salt
with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 47882-79-1

CMF C45 H33 O6 Si

CCI CCS

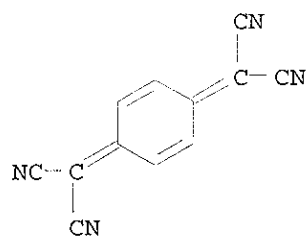


CM 2

CRN 34507-61-4

CMF C12 H4 N4

CCI RIS



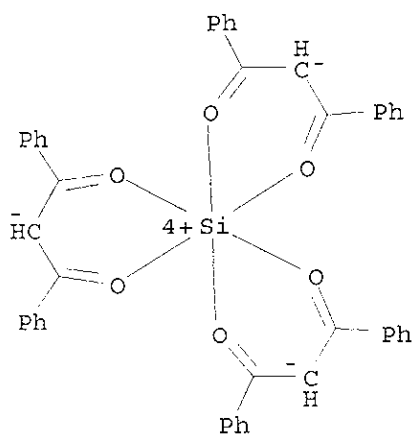
IT 12121-05-0 16871-35-5 36247-99-1

73881-84-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with lithiated TCNQ radical)

RN 12121-05-0 CAPLUS

CN Silicate(1-), tris(1,3-diphenyl-1,3-propanedionato-O,O')-, chloride,
(OC-6-11)- (9CI) (CA INDEX NAME)



RN 16871-35-5 CAPLUS

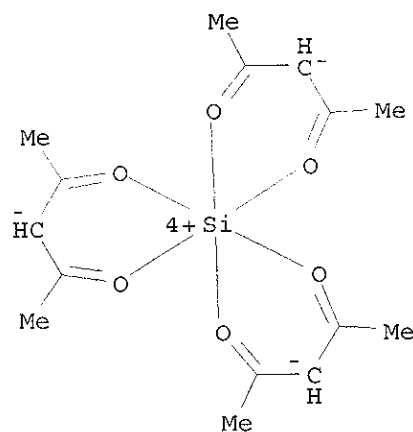
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, (hydrogen dichloride) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS

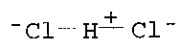


CM 2

CRN 23231-72-3

KOROMA EIC1700

CMF C12 H



RN 36247-99-1 CAPLUS

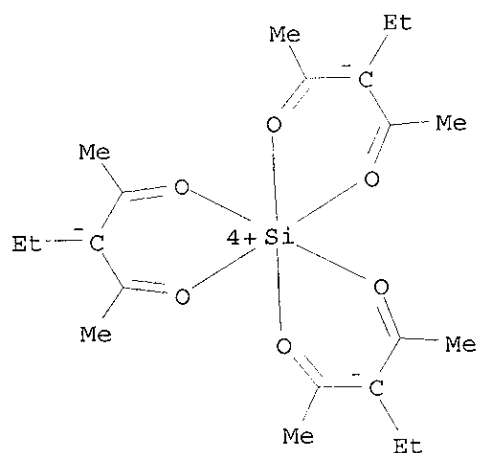
CN Silicon(1+), tris(3-ethyl-2,4-pentanedionato-O,O')-, (OC-6-11)-, (hydrogen dichloride) (9CI) (CA INDEX NAME)

CM 1

CRN 47559-76-2

CMF C21 H33 O6 Si

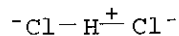
CCI CCS



CM 2

CRN 23231-72-3

CMF C12 H



RN 73881-84-2 CAPLUS

CN Silicon(1+), tris(2,2,6,6-tetramethyl-3,5-heptanedionato-O,O')-, (OC-6-11)-, (hydrogen dichloride) (9CI) (CA INDEX NAME)

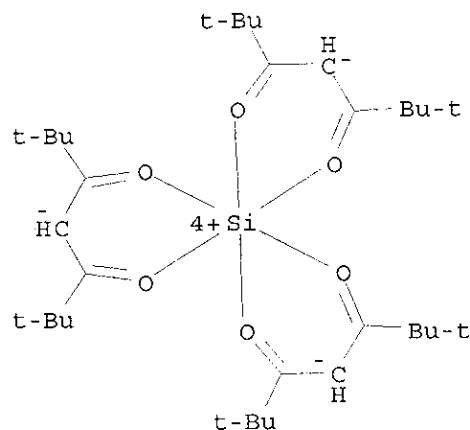
CM 1

CRN 73881-83-1

CMF C33 H57 O6 Si

KOROMA EIC1700

CCI CCS



CM 2

CRN 23231-72-3

CMF C12 H

$^{-}\text{Cl}-\text{H}^{+}\text{Cl}^{-}$

- CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
- ST **siliconium** trisdiketonato TCNQ salt; TCNQ radical anion
trisdiketonatosiliconium salt; crystal structure
trisacetylacetonatosiliconium TCNQ salt
- IT Crystal structure
Molecular structure
(of TCNQ radical anion-tris(acetylacetonato)**siliconium** salt
polymorphs)
- IT **Electric** resistance
(resistivity, of TCNQ radical anion-tris(diketonato)**siliconium**
salts)
- IT 97501-23-0P 97501-26-3P 97501-27-4P
97501-29-6P 97501-30-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and elec. resistivity of)
- IT 97501-24-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, elec. resistivity, and crystal and mol. structure of
2 crystalline forms of)
- IT 97501-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, elec. resistivity, and reaction of, with TCNQ)

KOROMA EIC1700

IT 1283-90-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(diketonato)siliconium compds.)
IT 12121-05-0 16871-35-5 36247-99-1
73881-84-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with lithiated TCNQ radical)
IT 1518-16-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with siliconium salt of radical ion of)

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1970:471846 CAPLUS

DOCUMENT NUMBER: 73:71846

TITLE: Electric-field effects in nuclear magnetic
resonance spectroscopy. III. ^{13}C -- ^1H spin-spin
coupling constants

AUTHOR(S): Hammel, J. C.; Smith, John A. S.

CORPORATE SOURCE: Sch. Mol. Sci., Univ. Warwick, Coventry, UK

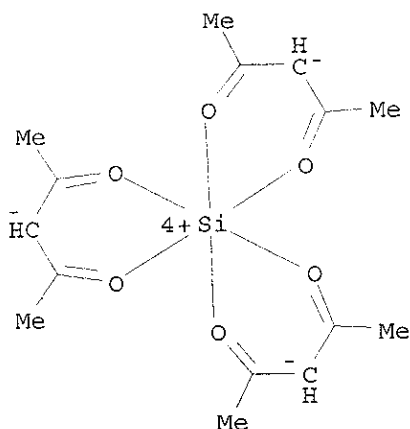
SOURCE: Journal of the Chemical Society [Section] A:
Inorganic, Physical, Theoretical (1970), (11), 1852-4
CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal

LANGUAGE: English

AB If the linear elec.-field dependence of the ^{13}C - ^1H spin-spin
coupling consts. in polar acetylacetonato complexes is assumed to depend
on the different elec. field at both the ^{13}C and ^1H nucleus,
then effects at ^1H are shown to be predominant. Previous empirical
equations giving the quant. dependence of the coupling constant on
elec. field are revised and shown to be consistent with theory.
When elec.-field effects are important, there is also a linear
relation between the ^1H and ^{13}C shifts and the corresponding ^{13}C - ^1H
coupling constant for both the Me and methine groups.

IT 23683-85-4
RL: PRP (Properties)
(nuclear magnetic resonance of, elec. field effects on)
RN 23683-85-4 CAPLUS
CN Silicon(1+), tris(2,4-pentanedionato- $\kappa\text{O},\kappa\text{O}'$)-, (OC-6-11)-
(9CI) (CA INDEX NAME)



- CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
- ST carbon 13 proton coupling consts; proton carbon 13 coupling consts; spin spin coupling consts; coupling consts spin spin; **elec** field effects NMR; NMR **elec** field effects; field **elec** effects NMR; acetylacetonate complexes polar NMR
- IT Nuclear magnetic resonance
(of pentanedione complexes, **elec.** field dependence of carbon-13-proton coupling constant in)
- IT **Electric** field, chemical and physical effects
(on nuclear spin-spin coupling, of carbon-13 with hydrogen)
- IT 2,4-Pentanedione, complexes
2,4-Pentanedione, 3-methyl-, boron complexes
RL: PRP (Properties)
(nuclear magnetic resonance of, **elec.** field effects on)
- IT 14947-58-1 15390-25-7 16919-65-6 29934-23-4 30085-15-5
RL: PRP (Properties)
(nuclear magnetic resonance of, **elec.** field effect on carbon-13-hydrogen spin-spin coupling in relation to)
- IT 23683-85-4
RL: PRP (Properties)
(nuclear magnetic resonance of, **elec.** field effects on)
- IT 1333-74-0, properties
RL: PRP (Properties)
(nuclear spin-spin coupling of, with carbon-13, **elec.** field effect on)
- IT 14762-74-4, properties
RL: PRP (Properties)
(nuclear spin-spin coupling of, with hydrogen, **elec.** field effects on)

L15 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1970:37559 CAPLUS
DOCUMENT NUMBER: 72:37559
TITLE: **Electric** field effects in magnetic

resonance. I. Carbon-13 chemical shifts
 AUTHOR(S): Hammel, J. C.; Smith, John Alec Sydney
 CORPORATE SOURCE: Sch. Med. Sci., Univ. Warwick, Coventry, UK
 SOURCE: Journal of the Chemical Society [Section] A:
 Inorganic, Physical, Theoretical (1969), (19), 2883-7
 CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The ^{13}C NMR spectra of 19 complexes of acetylacetone have been recorded and are compared with their ^1H spectra and the ir stretching frequencies of the ring atoms. The ^{13}C shifts of the Me and ring CH groups for 1st- and 2nd-row elements are explained largely in terms of 1st-order elec. field shifts, the coeffs. of proportionality between the ^{13}C and ^1H shifts being about -4.2 for Me and +0.94 for CH. The CO ^{13}C shifts appear to be related to the C:O and C:C ir stretching frequencies. Serious deviations from these generalizations are observed for elements with filled or partly filled d orbitals.

IT 16871-35-5

RL: PRP (Properties)

(nuclear magnetic resonance of, in presence of elec. field)

RN 16871-35-5 CAPLUS

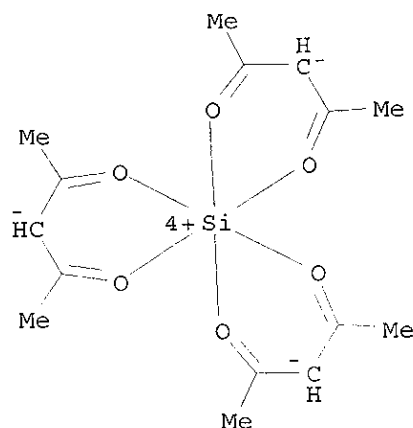
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, (hydrogen dichloride) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

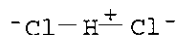
CCI CCS



CM 2

CRN 23231-72-3

CMF C12 H



- CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
- ST **elec** field effects NMR; NMR **elec** field effects; field **elec** effects NMR; carbon 13 chem shifts; chem shifts C 13; shifts chem C 13
- IT Nuclear magnetic resonance
(of carbon-13, in metal acetylacetonate complexes, **elec.** field effect on)
- IT **Electric** field, chemical and physical effects
(on nuclear magnetic resonance, of metal acetylacetonate complexes)
- IT 2,4-Pentanedione, metal complexes
Thallium, diethyl(2,4-pentanedionato)-
RL: PRP (Properties)
(nuclear magnetic resonance of, in presence of **elec.** field)
- IT 14762-74-4, properties
RL: PRP (Properties)
(nuclear magnetic resonance of, in metal acetylacetonate complexes, **elec.** field effect on)
- IT 123-54-6, properties 10210-64-7 13501-17-2 13963-57-0 14024-56-7
14405-43-7 14405-45-9 15350-61-5 15390-25-7 15435-71-9
16871-35-5 16919-46-3 17499-48-8 17501-44-9 18115-70-3
19372-44-2 19393-11-4 19426-80-3 21679-46-9
RL: PRP (Properties)
(nuclear magnetic resonance of, in presence of **elec.** field)

L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1968:501562 CAPLUS

DOCUMENT NUMBER: 69:101562

TITLE: Ring currents in metal acetylacetonates.
Electric field effects on the proton resonances of cationic and anionic β -diketonate complexes

AUTHOR(S): Fay, Robert C.; Serpone, Nick

CORPORATE SOURCE: Cornell Univ., Ithaca, NY, USA

SOURCE: Journal of the American Chemical Society (1968),
90(21), 5701-6
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Proton chemical shifts were measured in $CDCl_3$ solution for a series of cationic acetylacetonato complexes of the types $[M(acac)_3]X$ and $[B(acac)_2]X$ ($M = Si, Ge, \text{ and } Ti; X^- = Cl^-, Br^-, HCl_2^-, ClO_2^-, I_3^-, AuCl_4^-, \text{ or } SbCl_6^-$) and for the anionic benzoylacetonato and trifluoroacetylacetonato complexes, $[C_5H_{12}N][M(bzac)_4]$ and $[C_5H_{12}N][M(tfac)_4]$ ($M = La \text{ and } Y$). Some of these compds. have not been reported previously. The methyl and ring proton ($-CH=$) resonances of the cationic complexes are shifted downfield relative to the resonances of analogous, neutral metal diketonates,

whereas the resonances of the anionic complexes are shifted upfield. The observed shifts are examined in relation to the charge on the ion and the hypothesis of benzenoid ring currents. Point charge model calcns. indicate that the shifts can be satisfactorily accounted for in terms of the elec. field caused by the charge on the ion, and there is no need to invoke ring currents. The -CH = resonances of the cationic complexes depend on the size of the anion and the solution concentration; these dependences are discussed in terms of ion pairing.

IT 16871-35-5 16903-06-3 19552-36-4
21724-00-5

RL: PRP (Properties)

(nuclear magnetic resonance of, ring currents in relation to)

RN 16871-35-5 CAPLUS

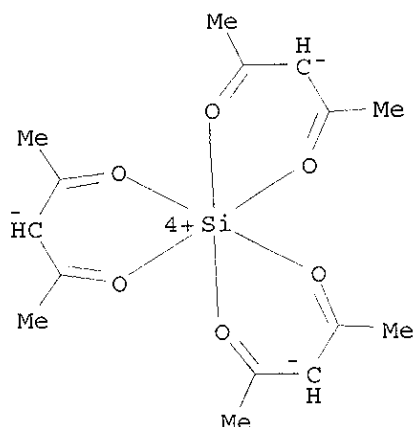
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, (hydrogen dichloride) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS



CM 2

CRN 23231-72-3

CMF C12 H

-Cl-H⁺ Cl⁻

RN 16903-06-3 CAPLUS

CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, (OC-6-11)-hexachloroantimonate(1-) (9CI) (CA INDEX NAME)

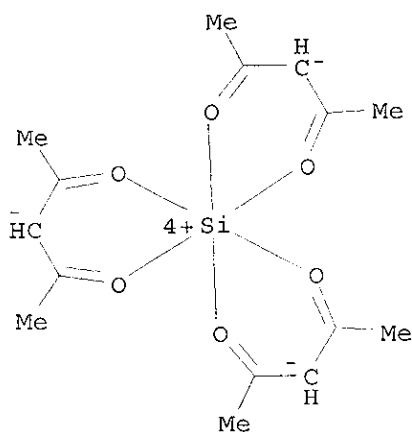
KOROMA EIC1700

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

CCI CCS

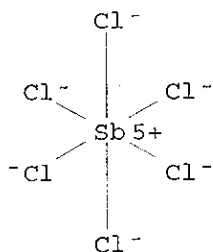


CM 2

CRN 17949-89-2

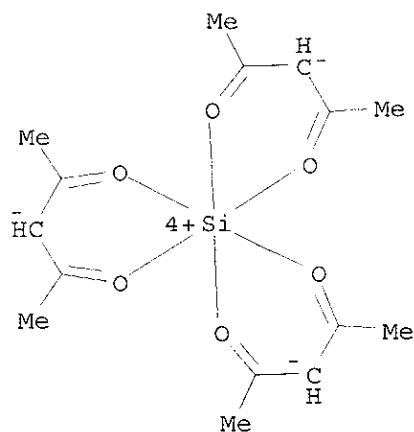
CMF Cl6 Sb

CCI CCS



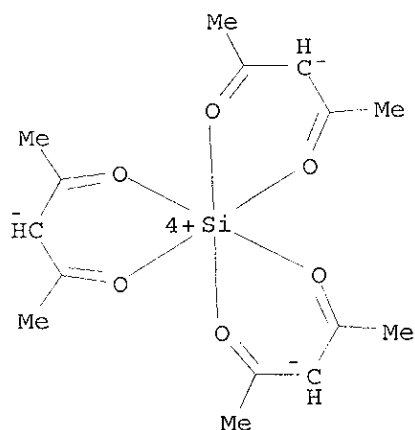
RN 19552-36-4 CAPLUS

CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, chloride, (OC-6-11)- (9Cl)
(CA INDEX NAME)



● Cl⁻

RN 21724-00-5 CAPLUS
 CN Silicon(1+), tris(2,4-pentanedionato)-, bromide (8CI) (CA INDEX NAME)



● Br⁻

CC 73 (Spectra and Other Optical Properties)
 ST acetylacetonates ring currents; ring currents acetylacetonates; currents
 ring acetylacetonates; chem shifts acetylacetonates; **silicon**
 acetylacetonates; germanium acetylacetonates; titanium acetylacetonates;
 benzoylacetate complexes; fluoroacetylacetonate complexes
 IT Nuclear magnetic resonance
 (of metal acetylacetonates, π -electron configuration in relation to)

KOROMA EIC1700

IT Electron configuration
 (π -, of metal acetylacetonates)
 IT 1,3-Butanedione, 1-phenyl-, metal complexes
 2,4-Pentanedione, metal complexes
 2,4-Pentanedione, 1,1,1-trifluoro-, complexes with lanthanum and yttrium
 RL: PRP (Properties)
 (N.M.R. and ring currents of)
 IT 16871-35-5 16903-05-2 16903-06-3 16903-07-4
 18924-18-0 19552-36-4 21608-50-4 21723-99-9
 21724-00-5 21724-03-8 21724-04-9 21793-26-0 21793-27-1
 21793-28-2 23336-07-4
 RL: PRP (Properties)
 (nuclear magnetic resonance of, ring currents in relation to)

L15 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1968:74753 CAPLUS

DOCUMENT NUMBER: 68:74753

TITLE: Preparation and properties of some six- and seven-coordinate halo(acetylacetonato) complexes of zirconium(IV) and hafnium(IV)

AUTHOR(S): Pinnavaia, Thomas J.; Fay, Robert C.

CORPORATE SOURCE: Cornell Univ., Ithaca, NY, USA

SOURCE: Inorganic Chemistry (1968), 7(3), 502-8

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

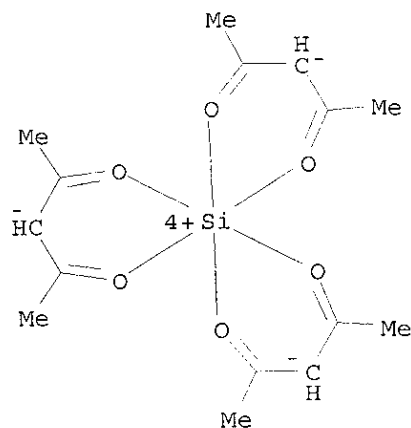
AB The preparation and characterization are reported of dihalobis(acetylacetonato) and halotris(acetylacetonato) complexes of Zr(IV) and Hf(IV), $M(\text{acac})_2X_2$ ($X = \text{Cl}$ or Br) and $M(\text{acac})_3X$ ($X = \text{Cl}$, Br , or when $M = \text{Zr}$, I). The Zr and Hf compds. containing the same halogen are isomorphous. The dihalides are monomeric weak electrolytes in solution; N.M.R. chemical shifts suggest that these complexes exist as cis geometrical isomers. The monohalides are monomeric seven-coordinate complexes which are only very slightly dissociated in ionizing solvents when $X = \text{Cl}$ or Br , but which are appreciably dissociated when $X = \text{I}$. The dissociated species of the monoiodide are markedly stabilized by tetrahydrofuran. N.M.R. spectra indicate that chelate rings in the halo and dihalo complexes undergo rapid configurational rearrangements; time-averaged spectra were observed even at temps. as low as -130° . Proton chemical shifts are reported and discussed in terms of the intramol. elec. field of the complexes and dipole-induced dipole interactions between the complexes and the solvent. 34 references.

IT 19552-36-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 19552-36-4 CAPLUS

CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, chloride, (OC-6-11)- (9CI)
 (CA INDEX NAME)



● Cl⁻

CC 78 (Inorganic Chemicals and Reactions)
 ST ZIRCONIUM COMPLEXES; HAFNIUM COMPLEXES; ACETYLACETONATO COMPLEXES
 IT Rearrangements
 (in 2,4-pentanedione complexes with hafnium and zirconium)
 IT Nuclear magnetic resonance
 (of 2,4-pentanedione complexes of hafnium and zirconium)
 IT Coordination numbers
 (seven, in 2,4-pentanedione complexes with hafnium and zirconium)
 IT 2,4-Pentanedione, metal complexes
 Furan, tetrahydro-, zirconium complex
 Hafnium, dibromobis(2,4-pentanedionato)-
 Zirconium, dibromobis(2,4-pentanedionato)-
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 16903-07-4P 17192-26-6P 17211-55-1P 17475-67-1P 17501-44-9P
 18717-38-9P 18726-64-2P 19439-87-3P 19552-35-3P 19552-36-4P
 19568-99-1P 19610-19-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1967:24208 CAPLUS
 DOCUMENT NUMBER: 66:24208
 TITLE: Nuclear magnetic resonance spectra of some
 β-diketone complexes of Groups III and IV
 elements
 AUTHOR(S): Smith, John A. S.; Wilkins, E. J.
 CORPORATE SOURCE: Univ. Warwick, Coventry, UK
 SOURCE: Journal of the Chemical Society [Section] A:
 Inorganic, Physical, Theoretical (1966), (12), 1749-57
 CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The chemical shifts of the CH and CH₃ protons in the N.M.R. spectra of many neutral β -diketone complexes are sensitive to the elec. symmetry of the mol. The effects are ascribed largely to intramol. linear elec.-field shifts and can be calculated from the dipole moment of the mol. The signs of the shifts can be used in discussing the structure of the complexes; they confirm the cis configuration for Ti(IV), Ge(IV), and Sn(IV) complexes of the type M(acac)₂Cl₂ (where acac = acetylacetonate), and the existence of 2 C-bonded (acac) ligands in [Pt(acac)₃]⁻. The large low-field shift of CH recently observed in [Si(acac)₃]⁺ is also ascribed to both 1st- and 2nd-order elec.-field shifts rather than to any marked benzenoid resonance in the β -diketone ring. 41 references.

IT 16871-35-5 16921-33-8 16921-34-9

RL: PRP (Properties)
 (N.M.R. of)

RN 16871-35-5 CAPLUS

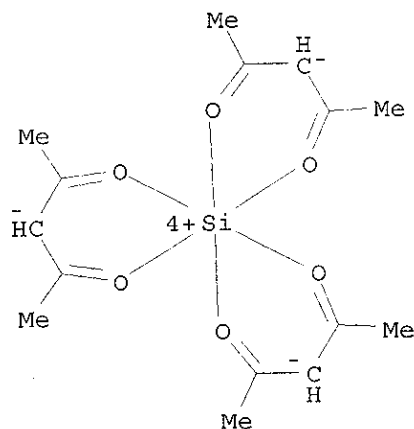
CN Silicon(1+), tris(2,4-pentanedionato-O,O')-, (OC-6-11)-, (hydrogen dichloride) (9CI) (CA INDEX NAME)

CM 1

CRN 23683-85-4

CMF C15 H21 O6 Si

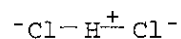
CCI CCS



CM 2

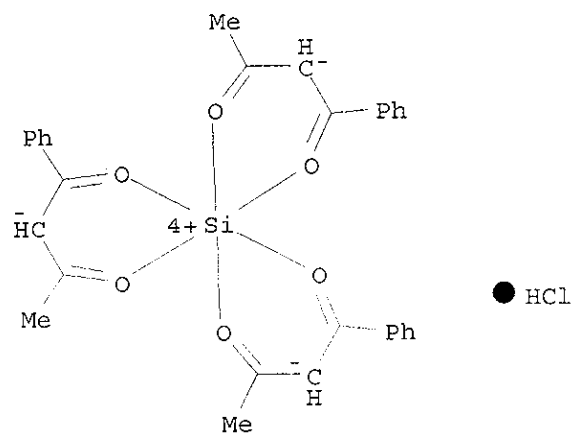
CRN 23231-72-3

CMF C12 H



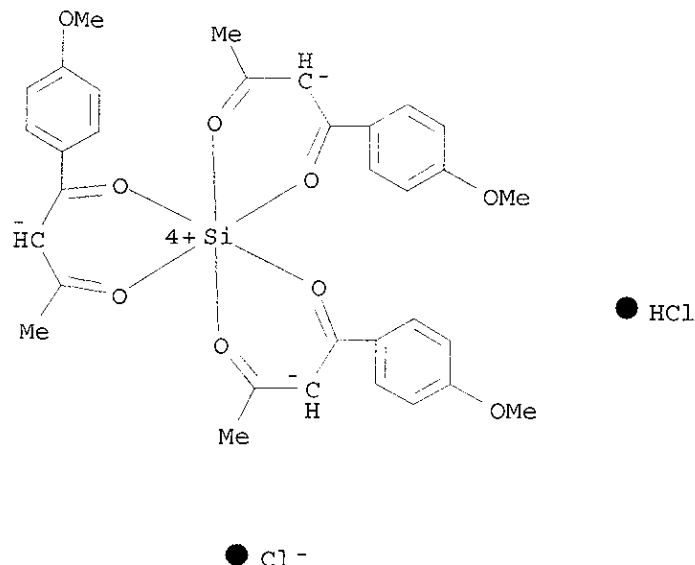
RN 16921-33-8 CAPLUS

CN Silicon(1+), tris(1-phenyl-1,3-butanedionato)-, hydrogen dichloride (8CI)
(CA INDEX NAME)



RN 16921-34-9 CAPLUS

CN Silicon(1+), tris[1-(p-methoxyphenyl)-1,3-butanedionato]-, hydrogen
dichloride (8CI) (CA INDEX NAME)



- CC 73 (Spectra and Other Optical Properties)
- ST NMR DIKETONE COMPLEXES; DIKETONE COMPLEXES NMR; TITANIUM 4 ACETONYLACETONATE NMR; GERMANIUM 4 ACETONYLACETONATE NMR; TIN 4 ACETONYLACETONATE NMR; ACETONYLACETONATE COMPLEXES NMR
- IT Nuclear magnetic resonance
(of β -diketone complexes of Groups III and IV elements)
- IT 2,4-Pentanedione, ion(1-), lithium
2,4-Pentanedione, 3-chloro-, metal complexes
2,4-Pentanedione, 3-methyl-, metal complexes
RL: PRP (Properties)
(N.M.R. of)
- IT 1,3-Butanedione, 1-(p-methoxyphenyl)-, complexes with boron
1,3-Butanedione, 1-phenyl-, complexes with boron
1,3-Propanedione, 1,3-diphenyl-, complexes with boron
2,4-Pentanedione, complexes with boron
RL: PRP (Properties)
(metals or silicon, N.M.R. of)
- IT Germanium, dichlorobis(2,4-pentanedionato)-
Tin, dichlorobis(2,4-pentanedionato)-
Tin, diiodobis(2,4-pentanedionato)-
Tin, tetrachlorobis(phenalen-1-one)-
RL: PRP (Properties)
(nuclear magnetic resonance of)
- IT 15435-71-9 16871-35-5 16921-33-8 16921-34-9
19393-11-4
RL: PRP (Properties)
(N.M.R. of)
- IT 1522-20-9 10210-64-7 13963-57-0 14024-56-7 14024-63-6 14219-90-0
14284-92-5 14354-58-6 14376-06-8 14405-36-8 14405-38-0
14405-39-1 14405-40-4 14405-41-5 14405-43-7 14405-45-9
14871-98-8 14947-58-1 14947-59-2 14947-61-6 15350-61-5

Page 45Toomer018

16894-10-3	16894-11-4	16919-46-3	17362-81-1	17475-67-1
17499-48-8	17501-44-9	17569-18-5	19033-51-3	19033-52-4
21679-46-9	65137-04-4			

RL: PRP (Properties)

(nuclear magnetic resonance of)

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